

The Density Functional via Effective Action

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A rigorous derivation of the density functional via the effective action in the Hohenberg-Kohn theory is outlined. Using the auxiliary field method, in which the electric coupling constant e^2 need not be small, we show that the loop expansion of the exchange-correlation functional can be reorganized so as to be expressed entirely in terms of the Kohn-Sham single-particle orbitals and energies.

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Interactions among electrons largely determine the structure, phases, and stability of matter. Pragmatic advances in this subject, however, are nontrivial. When the number of electrons involved becomes large, calculations based on constructing many-electron wave functions soon lose accuracy and will be stopped by an “exponential wall” [1]. Density functional theory (DFT), using the three-dimensional electronic density as the basic variable, is free from this wall. DFT originated from the theorem of Hohenberg and Kohn (HK) [2], which states that there exists a *unique* description of a many-body system in its ground state in terms of the expectation value of the particle-density operator. The HK theorem assures that the ground state energy E_g is obtained by minimizing the energy functional E_v with respect to the electronic density n :

$$E_g = \min_n E_v[n]. \quad (1)$$

Mermin [3] extended this theorem to finite-temperature.

To make practical use of the HK theorem, a suitable computational scheme is necessary. Kohn and Sham [4] proposed a decomposition scheme, aiming to express $E_v[n]$ via an auxiliary, *noninteracting* system that yields a particle density identical to that of the physical ground state. For a nonrelativistic fermion system described by

$$\hat{H} = \int d\mathbf{x} \hat{\psi}^\dagger(\mathbf{x}) \left(-\frac{1}{2m} \nabla^2 + v(\mathbf{x}) - \mu \right) \hat{\psi}(\mathbf{x}) + \frac{e^2}{2} \int \int \frac{\hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}^\dagger(\mathbf{y}) \hat{\psi}(\mathbf{y}) \hat{\psi}(\mathbf{x})}{|\mathbf{x} - \mathbf{y}|} d\mathbf{x} d\mathbf{y}, \quad (2)$$

the energy functional, with e^2 representing the electric coupling constant and $T_0[n]$ being the kinetic energy of the auxiliary system, takes the form

$$E_v[n] = \int v(\mathbf{x}) n(\mathbf{x}) d\mathbf{x} - \mu N_e + T_0[n] + \frac{e^2}{2} \int \int \frac{n(\mathbf{x}) n(\mathbf{y})}{|\mathbf{x} - \mathbf{y}|} d\mathbf{x} d\mathbf{y} + E_{xc}[n], \quad (3)$$

where μ = chemical potential, N_e = number of electrons, $v(\mathbf{x})$ = external potential, and $E_{xc}[n]$ is the so-called exchange-correlation energy functional. This *exact* decomposition cannot exist without the quantity $\frac{\delta E_{xc}[n]}{\delta n}$

being well defined. Being independent of $v(\mathbf{x})$, the sum of the last three terms in (3) is universal. All of the many-particle complexity is now completely hidden in $E_{xc}[n]$.

Although $T_0[n] + E_{xc}[n]$ admits no free parameter and is universal [2], its explicit construction remains elusive, and parameter-containing *empirical* functionals are therefore introduced. Cases of failure and limitations of these empirical functionals have been discussed [5, 6]. On the other hand, a number of groups [7, 8, 9, 10] have pursued first-principle derivation of the density functional via effective action. These efforts either introduce an auxiliary field [7, 10] or expand in powers of e^2 [8, 9]. The strengths of the auxiliary field approach are the simplicity of the effective action expression and the fact that each term already includes infinitely many Feynman diagrams [11]. However, this approach seems [7] to lack a direct connection to the Kohn-Sham (KS) scheme. Such a connection can be made in the expansion in powers of e^2 [9, 12], but that expansion is good only when e^2 is small [13]. The validity of that assumption depends on the strength and variation of $v(\mathbf{x})$.

In this Letter, without assuming e^2 small, we report our development [14] of an auxiliary field method that makes a direct connection to the KS scheme. To lighten the mathematical expressions in our finite-temperature formalism, we suppress the spin degree of freedom (as it is easy to include) and denote by a dot (circle) the three (four) dimensional integral contraction (with τ denoting the Euclidean time, $x \equiv (\tau, \mathbf{x})$)

$$a \cdot b \equiv \int d\mathbf{x} a(\mathbf{x}) b(\mathbf{x})$$

$$a \circ b \equiv \int d\tau d\mathbf{x} a(\tau, \mathbf{x}) b(\tau, \mathbf{x}) \equiv \int dx a(x) b(x).$$

To probe the electron density, one introduces to \hat{H} a classical source term $J(\mathbf{x})$ coupled to $\hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}(\mathbf{x})$, $\hat{H} \rightarrow \hat{H} + J \cdot (\hat{\psi}^\dagger \hat{\psi}) \equiv \hat{H}_J$. Let β be the temperature inverse, $\beta J \cdot (\hat{\psi}^\dagger \hat{\psi})$ is written as $J \circ (\hat{\psi}^\dagger \hat{\psi}) = \int dx J(x) \hat{\psi}^\dagger(x) \hat{\psi}(x)$. The partition function now is a functional of J , that is

$$Z[J] \Rightarrow e^{-\beta W[J]} = \text{Tr} \left[e^{-\beta [\hat{H} + J \cdot (\hat{\psi}^\dagger \hat{\psi})]} \right] \equiv \text{Tr} \left[e^{-\beta \hat{H}_J} \right]. \quad (4)$$

To disentangle the quartic fermionic interaction, we use the standard procedure of introducing an auxiliary

field ϕ and express $Z[J]$ as a path integral over both the Grassmann fields and the auxiliary field

$$e^{-\beta W[J]} = \int D\phi D\psi^\dagger D\psi e^{-S[\phi, \psi^\dagger, \psi]}, \quad (5)$$

where

$$S[\phi, \psi^\dagger, \psi] = -\frac{1}{2}\text{Tr} \ln(u) + \frac{1}{2}\phi \circ u \circ \phi + \psi^\dagger \circ G^{-1} \circ \psi \quad (6)$$

$$G^{-1}(x, x') = \left(\partial_\tau + \hat{h}(\mathbf{x}) + i(u \circ \phi)_x + J(x) \right) \delta(x - x') \quad (7)$$

$$\hat{h}(\mathbf{x}) = -\frac{\nabla^2}{2m} + v_{\text{ion}}(\mathbf{x}) - \mu \quad (8)$$

$$u(x, x') = \delta(\tau - \tau') e^2 / |\mathbf{x} - \mathbf{x}'| \equiv \delta(\tau - \tau') u(\mathbf{x}, \mathbf{x}'), \quad (9)$$

with $\psi^{(\dagger)}$ denoting the Grassmann fields satisfying $\psi^{(\dagger)}(\beta, \mathbf{x}) = -\psi^{(\dagger)}(0, \mathbf{x})$. It is easy to verify that

$$\frac{\delta(\beta W[J])}{\delta J(x)} = \langle \hat{\psi}^\dagger(x) \hat{\psi}(x) \rangle_J = \langle \hat{n}(x) \rangle_J \equiv n_J(x). \quad (10)$$

Eq. (10) expresses n in terms of J . The effective action is defined as the Legendre transformation of $\beta W[J]$

$$\Gamma[n_J] \equiv \beta W[J] - J \circ n_J, \quad (11)$$

where the subscript J indicates that the domain of $\Gamma[n]$ is the set of density profiles reachable by varying J . Eq. (11) also leads to

$$\frac{\delta \Gamma[n]}{\delta n} = -J. \quad (12)$$

We now show that $E_v[n] = \lim_{\beta \rightarrow \infty} \frac{1}{\beta} \Gamma[n]$. Eq. (4) assures that at the zero temperature limit $W[J]$ is simply the ground state energy corresponding to \hat{H}_J . Evidently, when $J = 0$, $\lim_{\beta \rightarrow \infty} \frac{1}{\beta} \Gamma[n]|_{n=n_g} = W[J]|_{J=0} = E_g$ where E_g stands for the ground state energy corresponding to \hat{H} and n_g represents the electron density at the physical ($J = 0$) ground state. When $J \neq 0$, the corresponding electronic density n_J is different from n_g and $\lim_{\beta \rightarrow \infty} \frac{1}{\beta} \Gamma[n]|_{n=n_J}$ represents the expectation value of \hat{H} , calculated using the ground state wave function corresponding to a different Hamiltonian \hat{H}_J . Thus by the definition of the ground state, $\lim_{\beta \rightarrow \infty} \frac{1}{\beta} \Gamma[n]|_{n=n_J} > \lim_{\beta \rightarrow \infty} \frac{1}{\beta} \Gamma[n]|_{n=n_g}$. This means that $\lim_{\beta \rightarrow \infty} \frac{1}{\beta} \Gamma[n]$ reaches its minimum at n_g . Thus $\lim_{\beta \rightarrow \infty} \frac{1}{\beta} \Gamma[n]$ has all the properties attributed to the energy functional E_v in (1) and (3). Since the HK theorem states that this functional is unique, it must in fact be equal to $\lim_{\beta \rightarrow \infty} \frac{1}{\beta} \Gamma[n]$.

If we make a change of variable $\phi \rightarrow \phi + iu^{-1} \circ J$ in (5-7) and integrate over the Grassmann fields, we obtain

$$\begin{aligned} e^{-\beta W[J]} &\equiv e^{\frac{1}{2}J \circ u^{-1} \circ J} e^{-\beta W_\phi[J]} \\ &= e^{\frac{1}{2}J \circ u^{-1} \circ J} \int D\phi e^{-I[\phi] - iJ \circ \phi}, \end{aligned} \quad (13)$$

where

$$I[\phi] = -\frac{1}{2}\text{Tr} \ln(u) + \frac{1}{2}\phi \circ u \circ \phi - \text{Tr} \ln(G_\phi^{-1}), \quad (14)$$

and

$$G_\phi^{-1}(x, x') = \left(\partial_\tau + \hat{h}(\mathbf{x}) + i(u \circ \phi)_x \right) \delta(x - x'). \quad (15)$$

Eq. (13) implies that

$$\beta W[J] = \beta W_\phi[J] - \frac{1}{2}J \circ u^{-1} \circ J, \quad (16)$$

and thus the left-hand side of (10) can be expressed differently, leading to

$$n_J = i\varphi - u^{-1} \circ J, \quad (17)$$

where $i\varphi \equiv \delta(\beta W_\phi[J])/\delta J$. To evaluate βW_ϕ , we follow Jackiw [11] and let $\phi \rightarrow \phi + \varphi$ in (13-15). In particular, (15) is rewritten as

$$G_{\phi+\varphi}^{-1}(x, x') = G_\varphi^{-1}(x, x') + i\delta(x - x') (u \circ \phi)_x, \quad (18)$$

and one obtains [11]

$$\begin{aligned} \beta W_\phi[J] &= \frac{1}{2}\text{Tr} \ln(\tilde{D}^{-1} \circ u) + \frac{1}{2}\varphi \circ u \circ \varphi - \text{Tr} \ln(G_\varphi^{-1}) \\ &+ iJ \circ \varphi - \sum_{n=1}^{\infty} \frac{1}{n!} \left\langle \left[\sum_{k=3}^{\infty} I^{(k)}[\varphi] \circ b_1 \dots \circ b_k \right]^n \right\rangle_{\text{1PI, conn.}}, \end{aligned} \quad (19)$$

where the subscript “1PI, conn.” means to include only connected, one-particle-irreducible diagrams, $b \equiv u \circ \phi$,

$$\begin{aligned} \tilde{D}^{-1} &= u^{-1} - D, \\ D(x, y) &= G_\varphi(x, y) G_\varphi(y, x), \end{aligned}$$

and

$$\begin{aligned} I^{(k)}[\varphi] \circ b_1 \dots \circ b_k &\equiv \frac{(-1)^{k-1}}{k} \int dx_1 \dots dx_k \\ &G_\varphi(x_k, x_1) \dots G_\varphi(x_{k-1}, x_k) (ib(x_1)) \dots (ib(x_k)). \end{aligned} \quad (20)$$

Fukuda *et al.* [7] obtained an expression similar to (19) and used it to derive an effective action as a functional of φ . They also noted that this auxiliary field approach does not make a direct connection to the KS scheme.

Coming to the point of departure from typical auxiliary field approaches, we show below how an exact correspondence to the KS scheme can be made for the auxiliary field method by decomposing the source J in a particular way. Let us define a free fermion propagator \mathcal{G}_0 by

$$\mathcal{G}_0^{-1}(x, x') = \left[\partial_\tau + \hat{h}(\mathbf{x}) + J_0(x) \right] \delta(x - x'), \quad (21)$$

where J_0 is chosen (if $\frac{\delta E_{xc}[n]}{\delta n}|_{n_J}$ exists, J_0 exists and can be written [14] as $u \cdot n_J + \frac{\delta E_{xc}[n]}{\delta n}|_{n_J} + J$) such that

$$-\mathcal{G}_0(x, x) = n_J(x). \quad (22)$$

Eq. (22) demands that this non-interacting (KS) system have electron density, $-\mathcal{G}_0(x, x)$, identical to $n_J(x)$, the electronic density of the physical system (where Coulomb

interactions exist). In (19), each occurrence of $iu\phi$ through G_ϕ is to be replaced by $J + u\phi n_J$ (from (17)).

To bring out the KS scheme, we perform the following source decomposition

$$J[n] = (J_0[n] - u\phi n_J) + J'[n] \equiv \tilde{J}_0[n] + J'[n]. \quad (23)$$

Then from (15) and (17) we have

$$G_\phi^{-1}(x, x') = \mathcal{G}_0^{-1}(x, x') + J'(x)\delta(x - x'). \quad (24)$$

Although the source decomposition (23) is introduced here for the first time in the auxiliary field approach, a similar method was used in [8, 9] to perform perturbative calculations using e^2 as the expansion parameter.

Substituting (17) and (19) into (16), one obtains an expression for $\beta W[J]$, which, upon introducing a parameter λ (to be set = 1 in the end) to denote the loop order, has the form $\beta W[J] = \beta \tilde{W}_0[J] + \sum_{i=1}^{\infty} \lambda^i (\beta W_i[J + u\phi n_J])$, where in particular [14]

$$\beta \tilde{W}_0[J] = \beta W_0[J + u\phi n_J] - \frac{1}{2} n_J \circ u \phi n_J, \quad (25)$$

with $\beta W_0[J + u\phi n_J] = -\text{Tr} \ln(G_\phi^{-1})$.

To arrive at an expansion headed by $-\text{Tr} \ln(G_\phi^{-1})$ instead of $-\text{Tr} \ln(G_\phi^{-1})$, and containing the expression $W_l[J_0]$ instead of $W_l[J + u\phi n_J]$, we expand $W_l[J + u\phi n_J] = W_l[J_0 + J']$ in powers of J' (subscript l omitted in the equation below)

$$W = W[J_0] + \frac{\delta W[J_0]}{\delta J_0} \circ J' + \frac{1}{2} \frac{\delta^2 W[J_0]}{\delta J_0 \delta J_0} \circ J' \circ J' + \dots \quad (26)$$

The expression $W_l[J_0]$ means that J is replaced by \tilde{J}_0 but $u\phi n_J$ is kept unchanged.[14] With (26), we may express $\beta W[J]$ as a double series

$$\beta W[J] = \beta \tilde{W}_{00} + \beta \sum_{i,k} W_{ik} (1 - \delta_{i,0} \delta_{k,0}) J'^k \lambda^i, \quad (27)$$

where each W_{ik} involves the k 'th derivative of W_i . In particular, \tilde{W}_{00} is given by (with $n_J \rightarrow n$ hereafter)

$$\beta \tilde{W}_{00} = \beta W_{00} - \frac{1}{2} n \circ u \phi n = -\text{Tr} \ln(\mathcal{G}_0^{-1}) - \frac{1}{2} n \circ u \phi n, \quad (28)$$

and in view of (22) W_{01} is given by

$$\frac{\delta(\beta W_0[J_0])}{\delta J_0} = n = \frac{\delta(\beta \tilde{W}_{00}[\tilde{J}_0])}{\delta \tilde{J}_0}. \quad (29)$$

The second half of (29) suggests that we define

$$\tilde{\Gamma}_0[n] = \beta \tilde{W}_{00}[\tilde{J}_0] - \tilde{J}_0 \circ n, \quad (30)$$

the Legendre transformation of the zeroth order contribution from $\beta W[J]$ (in terms of J' and λ), leading to

$$\frac{\delta \tilde{\Gamma}_0[n]}{\delta n} = -\tilde{J}_0. \quad (31)$$

Comparing (31) with (12), we find

$$\frac{\delta(\Gamma[n] - \tilde{\Gamma}_0[n])}{\delta n} = -J'. \quad (32)$$

The idea now is to develop a series for $\Gamma[n]$ led by $\tilde{\Gamma}_0[n]$. Subtracting (30) from (11), we have

$$\Gamma[n] - \tilde{\Gamma}_0[n] = \beta W[J] - \beta \tilde{W}_{00}[\tilde{J}_0] - J' \circ n, \quad (33)$$

in which the last two terms on the right hand side exactly cancel the terms in \tilde{W}_{00} and W_{01} contributing to $\beta W[J]$. So the series for $\Gamma - \tilde{\Gamma}_0$ is just (27) with those two terms removed. Next we convert the double sum in (27) into a single sum by expanding J' as a series in λ . We write

$$J'[n] = \sum_{l=1}^{\infty} J_l[n] \lambda^l, \quad (34)$$

where the precise expressions for J_1, J_2, \dots are as yet undetermined since (34) is not a loop expansion. We substitute (34) formally into (33) and (27) to obtain a series

$$\Gamma[n] - \tilde{\Gamma}_0[n] = \sum_{l=1}^{\infty} \Gamma_l[n] \lambda^l, \quad (35)$$

in which each Γ_l is defined explicitly in terms of the J_k , $\beta W_{k \leq l}[J_0]$, and their derivatives. Because W_{01} is missing from (33), any occurrence of J_k is accompanied by at least one other factor $J_{k'}$ or else by an occurrence of some $W_{i>0}$, and hence by a power of λ higher than the k 'th. In other words, the expression for $\Gamma_{l \geq 1}$ involves only J_k with $k < l$. We finally remove the indeterminacy in (34) by imposing (32) to hold order by order in λ , leading to

$$\frac{\delta \Gamma_l[n]}{\delta n} = -J_l. \quad (36)$$

Since $\Gamma_{l \geq 1}$ involves only $J_{k < l}$, all the J_l and Γ_l can be found explicitly by applying (35) and (36) alternately. The first few expressions are $\Gamma_1 = \beta W_1[J_0] = -\frac{1}{2} \text{Tr} \ln(\tilde{\mathcal{D}}_{J \rightarrow \tilde{J}_0}^{-1} \circ u)$, $J_1 = -\frac{\delta(\beta W_1[J_0])}{\delta J_0} \circ \frac{\delta J_0}{\delta n}$, $\Gamma_2 = \beta W_2[J_0] + \frac{\delta(\beta W_1[J_0])}{\delta J_0} \circ J_1 + \frac{1}{2} J_1 \circ \frac{\delta^2(\beta W_0[J_0])}{\delta J_0 \delta J_0} \circ J_1$.

For an arbitrary J_0 , one will obtain a corresponding density \tilde{n} . The computation of $\frac{1}{\beta} \Gamma[n]$ using (30), (35) and (36) evaluates the energy functional at density \tilde{n} , which may or may not be the ground state density. To obtain the ground state density and the corresponding J_0 , one needs to solve at zero temperature limit the extremal equation $0 = \frac{\delta \Gamma[n]}{\delta n}$, which we turn to shortly.

To carry out the calculation of $\Gamma[n]$, we need to compute J_l (see (36)) via the functional derivative

$$\frac{\delta}{\delta n} = \left(\frac{\delta n}{\delta J_0} \right)^{-1} \circ \frac{\delta}{\delta J_0} \equiv D_0^{-1} \circ \frac{\delta}{\delta J_0}. \quad (37)$$

Diagrams corresponding to $\beta W_l[J_0]$ and their derivatives contain the u , \mathcal{G}_0 , and $\tilde{\mathcal{D}}_0 \equiv \tilde{\mathcal{D}}_{J \rightarrow \tilde{J}_0}$ propagators. It is

easy to show that one may express $\delta n(x)/\delta J_0(y)$ as

$$-\frac{\delta \mathcal{G}_0(x, x)}{\delta J_0(y)} = \mathcal{G}_0(x, y) \mathcal{G}_0(y, x) = D_{J \rightarrow \tilde{J}_0}(x, y) \quad (38)$$

and thus $D_0^{-1} = D_{J \rightarrow \tilde{J}_0}^{-1}$, which we call the inverse density correlator. The differentiation rules of \mathcal{G}_0 , \tilde{D}_0 , and D_0^{-1} with respect to J_0 can be expressed diagrammatically:

$$\begin{aligned} x' \cdots \cdots x & \quad u(x, x') & x' \longleftrightarrow x & \quad D_0^{-1}(x, x') \\ x' \longrightarrow x & \quad \mathcal{G}_0(x, x') & x' \text{---} \text{wavy} \text{---} x & \quad \tilde{D}_0(x, x') \\ \frac{\delta \mathcal{G}_0(x, x')}{\delta J_0(y)} = \frac{\delta}{\delta J_0(y)} & \quad \begin{array}{c} x \\ \uparrow \\ x' \end{array} & = - \begin{array}{c} x \\ \uparrow \\ y \\ \uparrow \\ x' \end{array} \\ \frac{\delta \tilde{D}_0(x, x')}{\delta J_0(y)} = \frac{\delta}{\delta J_0(y)} & \quad \begin{array}{c} x \\ \text{---} \text{wavy} \text{---} \\ x' \end{array} & = - \begin{array}{c} x \\ \text{---} \text{wavy} \text{---} y \\ \uparrow \\ x' \end{array} - \begin{array}{c} x \\ \text{---} \text{wavy} \text{---} y \\ \downarrow \\ x' \end{array} \\ \frac{\delta D_0^{-1}(x, x')}{\delta J_0(y)} = \frac{\delta}{\delta J_0(y)} & \quad \begin{array}{c} x \\ \text{---} \text{---} \text{---} \\ x' \end{array} & = + \begin{array}{c} x \\ \text{---} \text{---} \text{---} y \\ \uparrow \\ x' \end{array} + \begin{array}{c} x \\ \text{---} \text{---} \text{---} y \\ \downarrow \\ x' \end{array} . \end{aligned}$$

The differentiation rules of \mathcal{G}_0 , \tilde{D}_0 , and D_0^{-1} with respect to n are simply obtained by compounding the results above with (37). We show only one example:

$$\frac{\delta \mathcal{G}_0(x, x')}{\delta n(z)} = \frac{\delta}{\delta n(z)} \begin{array}{c} x \\ \uparrow \\ z \\ \uparrow \\ x' \end{array} = - \begin{array}{c} x \\ \text{---} \text{---} \text{---} z \\ \uparrow \\ x' \end{array} .$$

Equipped with these differentiation rules, one may use standard diagrammatic expansion to compute the $W_I[J_0]$ s, their functional derivatives with respect to J_0 , as well as J_I s to facilitate the calculations of Γ_I s. Because $D_0(x, y) = \mathcal{G}_0(x, y) \mathcal{G}_0(y, x)$, both $\tilde{D}_0 = (u^{-1} - D_0)^{-1}$ and D_0^{-1} can be expressed in terms of single-particle orbitals and energies through $\mathcal{G}_0(x, y)$ –the propagator of the KS system– which can be expressed as

$$\begin{aligned} \mathcal{G}_0(x, y) &= \sum_{\alpha} \phi_{\alpha}(\mathbf{x}) \phi_{\alpha}^*(\mathbf{y}) e^{-(\varepsilon_{\alpha} - \mu)(\tau_x - \tau_y)} \times \\ &\times \begin{cases} (-n_{\alpha}) & \text{if } \tau_x \leq \tau_y \\ (1 - n_{\alpha}) & \text{if } \tau_x > \tau_y \end{cases} , \end{aligned} \quad (39)$$

where $n_{\alpha} = 1/(e^{\beta(\varepsilon_{\alpha} - \mu)} + 1)$, $\sum_{\alpha} n_{\alpha} = N_e$, and the single particle orbital $\phi_{\alpha}(\mathbf{x})$ satisfies

$$[\hat{h}(\mathbf{x}) + J_0(\mathbf{x})] \phi_{\alpha}(\mathbf{x}) = (\varepsilon_{\alpha} - \mu) \phi_{\alpha}(\mathbf{x}) .$$

Since $\frac{\delta \tilde{\Gamma}_0[n]}{\delta n} = -\tilde{J}_0$, the extremal condition $0 = \frac{\delta \Gamma[n]}{\delta n}$ that determines n_g and $J_0[n_g]$ (as $\beta \rightarrow \infty$) becomes

$$\frac{\delta (\sum_{i=1}^{\infty} \Gamma_i[n])}{\delta n} = D_0^{-1} \circ \frac{\delta (\sum_{i=1}^{\infty} \Gamma_i[J_0[n]])}{\delta J_0} = \tilde{J}_0 . \quad (40)$$

Eq. (40) has to be solved self-consistently by keeping Γ_i terms up to some order in λ . Although a truncation is necessary, we note that each diagram in our expression already corresponds to infinitely many Feynman diagrams when using e^2 as the expansion parameter. This is easily seen by performing the small e^2 expansion of \tilde{D}_0

$$\tilde{D}_0 = u + u \circ D_0 \circ u + u \circ D_0 \circ u \circ D_0 \circ u + \dots ,$$

a sum of infinitely many (dressed) propagators. Interestingly, in the strong coupling limit where one must treat u^{-1} as a small parameter, we may express \tilde{D}_0 as

$$\tilde{D}_0 = -D_0^{-1} - D_0^{-1} \circ u^{-1} \circ D_0^{-1} - D_0^{-1} \circ u^{-1} \circ D_0^{-1} \circ u^{-1} \circ D_0^{-1} - \dots$$

while the traditional e^2 expansion fails completely.

Finally we sketch how (3) arises from $\Gamma[n]$. Eq. (30) may be rewritten as $\frac{1}{\beta} \tilde{\Gamma}_0[n] = \frac{1}{\beta} [-\text{Tr} \ln(\mathcal{G}_0^{-1}) - J_0 \circ n] + \frac{1}{2\beta} n \circ u \circ n$. Because $-\text{Tr} \ln(\mathcal{G}_0^{-1}) = \sum_{\alpha} \ln(1 - n_{\alpha})$, at zero temperature limit, the first two terms of $\frac{1}{\beta} \tilde{\Gamma}_0$ above give rise to the $T_0[n] - \mu N_e + \int v(\mathbf{x}) n(\mathbf{x}) d\mathbf{x}$ while the last part is exactly the Hartree term [14]. The exchange-correlation functional $E_{xc}[n]$ equals $\lim_{\beta \rightarrow \infty} \frac{1}{\beta} \sum_{i=1}^{\infty} \Gamma_i[n]$. We also comment that the excitations of the system can be studied [14] under this formalism and the energy functional shown in this letter has the correct single-electron limit [14].

Providing a scheme beyond perturbative expansion in e^2 , we have proposed an effective action construction that will contribute to the development of the parameter-free universal density functional.

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